

0.1 Molecular sets as representations of chemical reactions

A [uni-molecular chemical reaction](#) is defined by the [natural transformations](#)

$$\eta : h^A \longrightarrow h^B,$$

specified in the following [commutative diagram](#):

$$\begin{array}{ccc} h^A(A) = Hom(A, A) & \xrightarrow{\eta_A} & h^B(A) = Hom(B, A), \\ \downarrow h^A(t) & & \downarrow h^B(t) \\ h^A(B) = Hom(A, B) & \xrightarrow{\eta_B} & h^B(B) = Hom(B, B) \end{array} \quad (0.1)$$

with the [states of molecular sets](#) $A_u = a_1, \dots, a_n$ and $B_u = b_1, \dots, b_n$ being defined as the endomorphism sets $Hom(A, A)$ and $Hom(B, B)$, respectively. In general, *molecular sets* M_S are defined as finite sets whose elements are [molecules](#); the *molecules* are mathematically defined in terms of their molecular [observables](#) as specified next. In order to define molecular observables one needs to define first the [concept](#) of a [molecular class variable](#) or *m.c.v.*

A *molecular class variables* is defined as a family of molecular sets $[M_S]_{i \in I}$, with I being either an indexing set, or a proper class, that defines the variation range of the *m.c.v.* Most physical, chemical or biochemical applications require that I is restricted to a finite set, (that is, without any sub-classes). A [morphism](#), or molecular mapping, $M_t : M_S \rightarrow M_S$ of molecular sets, with $t \in T$ being real time values, is defined as a time-dependent mapping or [function](#) $M_S(t)$ also called a [molecular transformation](#), M_t .

An *m.c.v. observable* of B , characterizing the products of chemical [type](#) “B” of a chemical reaction is defined as a morphism:

$$\gamma : Hom(B, B) \longrightarrow \mathfrak{R},$$

where $\mathfrak{R}$ is the set or [field](#) of real numbers. This mcv-observable is subject to the following [commutativity](#) conditions:

$$\begin{array}{ccc} Hom(A, A) & \xrightarrow{f} & Hom(B, B) \\ \downarrow e & & \downarrow \gamma \\ Hom(A, A) & \xrightarrow{\delta} & R, \end{array} \quad (0.2)$$

with $c : A_u^* \longrightarrow B_u^*$, and A_u^* , B_u^* being, respectively, specially prepared *fields of states* of the molecular sets A_u , and B_u within a measurement uncertainty range, Δ , which is determined

by Heisenberg's uncertainty [relation](#), or the [commutator](#) of the observable [operators](#) involved, such as $[A^*, B^*]$, associated with the observable A of molecular set A_u , and respectively, with the observable B of molecular set B_u , in the case of a molecular set A_u interacting with molecular set B_u .

With these concepts and preliminary data one can now define the category of molecular sets and their transformations as follows.

0.2 Category of molecular sets and their transformations

Definition 0.1. The *category of molecular sets* is defined as the [category](#) C_M whose [objects](#) are molecular sets M_S and whose morphisms are molecular transformations M_t .

Remark 0.1. This is a mathematical [representation](#) of chemical reaction [systems](#) in terms of molecular sets that vary with time (or *msv*'s), and their transformations as a result of diffusion, [collisions](#), and chemical reactions.

[Classification](#): AMS MSC: 18D35 ([category theory](#); homological algebra :: [categories with structure](#) :: Structured objects in a category) 92B05 (Biology and other natural sciences :: Mathematical biology in general :: General biology and biomathematics) 18E05 (Category theory; homological algebra :: [abelian categories](#) :: Preadditive, [additive categories](#)) 81-00 ([quantum theory](#) :: General reference [works](#))

References

- [1] Bartholomay, A. F.: 1960. Molecular Set Theory. A mathematical representation for chemical reaction mechanisms. *Bull. Math. Biophys.*, **22**: 285-307.
- [2] Bartholomay, A. F.: 1965. Molecular Set Theory: II. An aspect of biomathematical theory of sets., *Bull. Math. Biophys.* **27**: 235-251.
- [3] Bartholomay, A.: 1971. Molecular Set Theory: III. The Wide-Sense Kinetics of Molecular Sets ., *Bulletin of Mathematical Biophysics*, **33**: 355-372.
- [4] Baianu, I. C.: 1983, Natural Transformation Models in Molecular Biology., in *Proceedings of the SIAM Natl. Meet.*, Denver, CO.; Eprint at cogprints.org with No. 3675.
- [5] Baianu, I.C.: 1984, A Molecular-Set-Variable Model of Structural and Regulatory Activities in Metabolic and Genetic Networks *FASEB Proceedings* **43**, 917.